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DSMC Implementation of Experimentally-Based $\text{Xe}^+ + \text{Xe}$ Differential Cross Sections for Electric Propulsion Modeling

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Abstract. Published differential cross section data for heavy particle collisions between xenon ions and neutral xenon has been incorporated into plasma simulations for electric propulsion modeling. A fit has been made to the published data in order to estimate the relative contribution from charge exchange and elastic collisions and to reduce the computational cost of utilizing the differential cross section in existing numerical models. Since the published profiles do not include scattering data near 0 degrees, the differential cross section was assumed to be constant at low angles. The angle at which the differential cross section was assumed to transition from the constant profile to the fit was chosen such that the differential cross section integrated to the published total cross section value for xenon scattering. In order to make the resulting differential scattering curve generally applicable to other types of collisions with dissimilar collision partners, the profile was converted from the laboratory frame into center of mass coordinates. Each time a scattering event was determined to take place in the electric propulsion modeling codes, a scattering angle of the incident particle was chosen using a cumulative distribution function. The behavior of the target particle was determined using conservation of energy and momentum.

Keywords: Plasma Simulation, Monte Carlo Methods, Electric Propulsion.

PACS: 52.65.Pp

INTRODUCTION

Large angle scattering of primary ions emitted from electric propulsion devices is a principal area of concern for spacecraft integration. Charge exchange or elastic collisions between high velocity ions and the slow plume of neutral gas trailing the spacecraft may result in contamination through sputtering and deposition. Until recently, the energy and angular dependence of the products of these types of collisions were unknown for the xenon propellant commonly used in electric propulsion devices such as Hall thrusters. Therefore, in the past, simple scattering models have been employed such as charge exchange collisions free of momentum transfer and elastic collisions resulting in isotropic scattering.

Recent measurements taken at Hanscom Air Force Base using a guided-ion beam experiment have resulted in the calculation of ion-atom interaction potentials for both single and doubly charged xenon ions [1]. These interaction potentials were used to compute the absolute differential cross section at a typical Hall thruster primary ion energy of 270 eV per unit charge. The new differential cross section data has been combined with previous measurements of total charge exchange cross sections and incorporated into the Draco module of the electric propulsion plume model, Coliseum, using a Monte Carlo collision technique [2]. For computational speed, a simple log-log form is fit to the differential cross section data and a cumulative distribution function is used to randomly choose the post-collision scattering angles. Post-collision velocities are determined based on conservation of energy and momentum. For greater flexibility in future simulations involving unlike collision partners, all collision-based computations were done in the center of mass reference frame and converted to a laboratory frame. This work discusses the details of implementation for the new collision model in the existing electric propulsion code.

DIFFERENTIAL CROSS SECTION

In Reference 1, the authors have experimentally measured the differential cross section of $\text{Xe}^+ + \text{Xe}$ and $\text{Xe}^{2+} + \text{Xe}$ at laboratory ion energies between 5 and 40 eV. They have used their results to derive interaction potentials which they have then used to calculate the absolute differential cross section at energies relevant to the electric propulsion device known as the Hall thruster. The results presented here are based on their calculation of the differential cross section at an ion energy per unit charge of 300 V. In order to make this data more computationally tractable in existing Monte Carlo collision methods, the following three steps have been performed:

1. Fitting a curve to published differential cross section data.
2. Determining a cutoff angle below which to assume differential cross section is constant.
3. Converting from the laboratory reference frame to the center of mass reference frame.

In order to reduce the computational cost of choosing a scattering angle, a fit has been used to characterize the differential cross section for each ion charge state. Noting that the published data is approximately linear on a log-log scale the following form has been selected:

$$\left. \frac{d\sigma}{d\Omega} \right|_{LAB} = \theta^{A_{-el}} 10^{B_{-el}} + (90 - \theta)^{A_{-ct}} 10^{B_{-ct}} \quad (1)$$

where θ is the laboratory scattering angle in degrees, $d\sigma/d\Omega$ is the differential cross section, and the subscript LAB denotes the laboratory reference frame. The above form has the added advantage that it separates the contributions of both elastic collisions and charge transfer collisions to the total differential cross section. The optimized coefficients are listed in Table 1 and a comparison between the published data and the curve fit is shown in Figure 1 for each charge state.

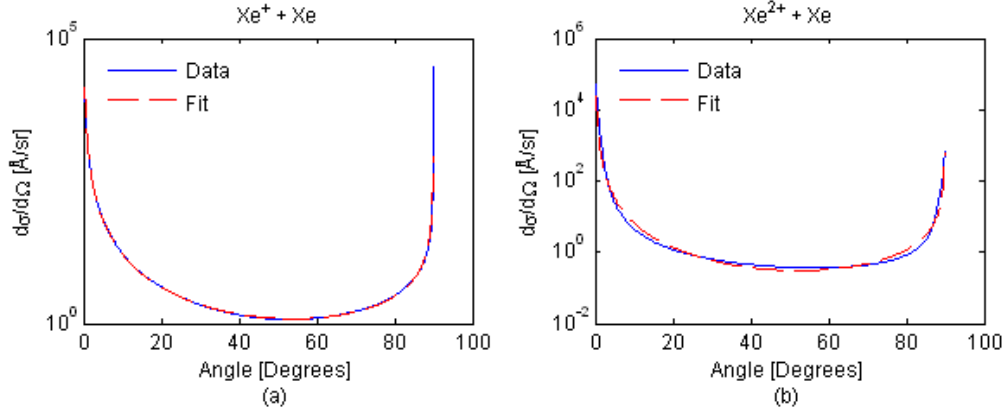


FIGURE 1. Comparison between published differential cross section data and optimized curve fit for (a) $\text{Xe}^+ + \text{Xe}$ and (b) $\text{Xe}^{2+} + \text{Xe}$.

TABLE 1. Coefficients used in curve fit to published data.

Coefficients	$\text{Xe}^+ + \text{Xe}$	$\text{Xe}^{2+} + \text{Xe}$
A_el	-2.02	-2.34
B_el	3.24	3.17
θ_el	0.0045	0.059
A_ct	-1.098	-1.43
B_ct	1.53	1.47
θ_ct	0.0022	0.143

The differential cross section data in Ref. [1] is only provided between the angles of 0.3 and 85.95 degrees. Since a significant amount of scattering occurs between 0 and 0.3 degrees and between 89.95 and 90 degrees, the differential cross section in this region must be specified. Note that the form of the curve fit specified by Eqn. (1) diverges at 0 and 90 degrees. Therefore, the differential cross section is assumed to reach a constant maximum value

at extreme angles. The angle at which the form transitions from Eqn. (1) to a constant value is given by θ_{el} for the elastic contribution and θ_{ct} for the charge transfer contribution. These angles are separately chosen such that the total cross section is given by the published charge transfer cross section specified in Ref. [3], namely 53.6 \AA^2 for $\text{Xe}^+ + \text{Xe}$ and 23.7 \AA^2 for $\text{Xe}^{2+} + \text{Xe}$. The total cross section, σ_{tot} , is calculated using the following formula:

$$\sigma_{tot} = \int_0^\pi \left. \frac{d\sigma}{d\Omega} \right|_{LAB} 2\pi \sin(\theta_{rad}) d\theta_{rad} \quad (2)$$

where θ_{rad} is the laboratory scattering angle in radians. When integrating over the charge transfer cross section, the angle in the integral is replaced with $(\pi/2 - \theta_{rad})$ since the laboratory scattering angle in this case is the recoil angle of the target particle which was initially neutral. The resulting values of θ_{el} and θ_{ct} are given in Table 1. Figure 2 demonstrates the constant assumed differential cross section for the elastic and charge transfer scattering of $\text{Xe}^+ + \text{Xe}$. Note that the elastic total cross section has been assumed to be equal to the charge transfer total cross section for each ion charge state.

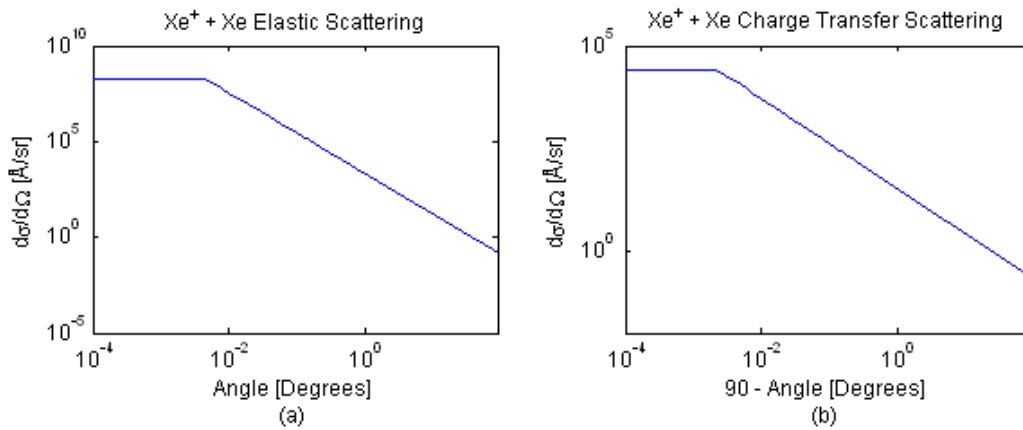


FIGURE 2. Assumed form of $\text{Xe}^+ + \text{Xe}$ differential cross section for (a) elastic and (b) charge transfer scattering.

For ease of conserving momentum and energy, as well as to generalize the resulting profiles to unequal collision partners, the differential cross section was converted from laboratory to center of mass coordinates using the following formulas for collision partners of equal weight:

$$\left. \frac{d\sigma}{d\Omega} \right|_{CM} = \left. \frac{d\sigma}{d\Omega} \right|_{LAB} \frac{1}{4 \cos \theta} \quad (3)$$

$$\chi = 2\theta \quad (4)$$

where χ is the center of mass scattering angle in degrees and the subscript „ CM “ indicates center of mass. Note that for charge transfer collisions, θ is replaced with $90 - \theta$.

In terms of the center of mass scattering angle, χ , rather than the solid angle, Ω , the differential cross section can be expressed as:

$$\frac{d\sigma}{d\chi} = \left. \frac{d\sigma}{d\Omega} \right|_{CM} 2\pi \sin \chi \quad (5)$$

Therefore, using the trigonometric identity, $\sin(2\theta) = 2 \cos(\theta) \sin(\theta)$, the differential cross section for elastic collisions is given by:

$$\frac{d\sigma}{d\chi} = \begin{cases} \left(\frac{\chi}{2}\right)^{A-el} 10^{B-el} \pi \sin\left(\frac{\chi}{2}\right) & \text{for } \chi \geq 2\theta_{-el} \\ (\theta_{-el})^{A-el} 10^{B-el} \pi \sin(\theta_{-el}) & \text{for } \chi < 2\theta_{-el} \end{cases} \quad (6)$$

For charge transfer collisions, the differential cross section is given by:

$$\frac{d\sigma}{d\chi} = \begin{cases} \left(\frac{\chi}{2}\right)^{A-ct} 10^{B-ct} \pi \cos\left(\frac{\chi}{2}\right) & \text{for } \chi \geq 2\theta_{-ct} \\ (\theta_{-ct})^{A-ct} 10^{B-ct} \pi \cos(\theta_{-ct}) & \text{for } \chi < 2\theta_{-ct} \end{cases} \quad (7)$$

MONTE CARLO METHODS

Several different methods are employed to incorporate heavy-particle collisions into the existing electric propulsion models. The first step in each method is determining which particles in the simulation should undergo a collision at each time step.

In the existing electric propulsion codes, the decision to perform a collision is determined by testing every ion particle individually. First, a collision partner is chosen randomly either by constructing a random particle using fluid background properties or by choosing a particle randomly from within the same cell. Using the properties of the ion being considered and the randomly chosen neutral partner, the probability of a collision is calculating using the following formula:

$$P = 1 - \exp(-n\sigma|\bar{c}_r|\Delta t) \quad (8)$$

where P is the probability of collision, n is the number density of the target species (neutrals in this case), c_r is the relative velocity, and Δt is the timestep. This probability is compared to a random number to determine whether or not a collision takes place.

Once it has been determined that a collision is statistically likely to occur and the collision partners have been chosen, the following steps are performed to execute the collision.

1. Choose center of mass scattering angles using statistical sampling.
2. Assuming pre-collision relative velocity is aligned along a principle direction, calculate post-collision relative velocity.
3. Rotate coordinate axes to account for actual direction of pre-collision relative velocity.
4. Convert from center of mass to laboratory reference frame.

In carrying out a collision, the first step is to use statistical sampling to determine the polar and azimuthal scattering angles. For convenience, it is easiest to align the pre-collision relative velocity along a principle direction, such as the z -axis as shown in Fig. 3 (a). Due to axisymmetry, the azimuthal scattering angle is chosen randomly from 0 to 2π . The polar scattering angle is chosen using the differential cross sections specified by Eqns. 6 and 7 depending on the collision type. For each type of collision, a comparison function is used to select a random angle from the distribution. Based on the form of the differential cross section, the comparison function chosen was:

$$f_t(\chi) = \begin{cases} \theta^A & \text{for } \chi \leq \theta \\ \chi^A & \text{for } \chi > \theta \end{cases} \quad (9)$$

where θ and A are the coefficients specific to each type of collision as listed in Table 1. In order to select a number randomly from this comparison function, a cumulative distribution function is used. The polar scattering angle, χ , is chosen such that:

$$\frac{\int_0^\chi f_i(\alpha) d\alpha}{\int_0^\pi f_i(\alpha) d\alpha} = \xi \quad (10)$$

where ξ is a random number between 0 and 1. An acceptance-rejection technique is then used to determine whether or not to select this value of χ or pick a new value. Based on the form of the differential cross section, the value selected is retained with probability $\sin(\chi/2)$ for elastic collisions and $\cos(\chi/2)$ for charge transfer collisions.

Once azimuthal scattering angle, ϕ , and polar scattering angle, χ , have been determined, the post-collision relative velocity in the z-aligned reference frame is computed using the following formulas:

$$\begin{aligned} c_{rx}^{z*} &= c_r^z \sin \chi \cos \phi \\ c_{ry}^{z*} &= c_r^z \sin \chi \sin \phi \\ c_{rz}^{z*} &= c_r^z \cos \chi \end{aligned} \quad (11)$$

where the subscript , r ' denotes relative velocity, the superscript , z ' denotes a z-axis aligned reference frame, and the superscript , $*$ ' denotes a post-collision velocity.

Since the above formulas assume that the initial relative velocity was aligned along a principle direction (the z-axis), a rotation must be performed on the resulting relative velocity vector to account for the actual orientation of the initial relative velocity vector. Assuming that the polar and azimuthal rotation angles are given by β and γ respectively, as shown in Fig. 3 (b), the following transformation yields the final relative velocity vector:

$$\beta = \tan^{-1} \left(\sqrt{c_x^2 + c_y^2} \right) \quad (12)$$

$$\gamma = \tan^{-1} \left(\frac{c_y}{c_x} \right) \quad (13)$$

$$\vec{c}_r^* = \begin{bmatrix} \cos \gamma & -\sin \gamma & 0 \\ \sin \gamma & \cos \gamma & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \cos \beta & 0 & \sin \beta \\ 0 & 1 & 0 \\ -\sin \beta & 0 & \cos \beta \end{bmatrix} \vec{c}_r^{z*} \quad (14)$$

Once the post-collision relative velocity has been determined in the center of mass frame, the final velocity vectors of each particle in the laboratory reference frame are calculated. If the collision type is elastic, these velocities are directly applied to the source and target particles. In the case of charge exchange collisions, the final velocity of the source particle is applied to the target particle and the final velocity of the target particle is applied to the source particle to reflect the transfer of charge that accompanies this type of collision.

TEST CASE

In order to test the functionality of the collision routine implemented in the electric propulsion plume model, COLISEUM, a simple test case was constructed in order to verify that the imposed differential cross section is correctly utilized by the code. The test case geometry, illustrated in Fig. 3(a), consists of a cylindrical beam impinging on a rectangular target box of neutral gas. The total domain size of the simulation is 10 cm x 10 cm x 2 cm with a cell spacing of 1 mm, resulting in 200,000 cells in total. The injector surface is a 10 mm diameter circle with a flow rate of Xe^+ of $2.78\text{e-}8$ kg/s. The directed energy of the beam is 300 eV, corresponding to a velocity of 21144 m/s, with a thermal energy component of 100K. Under these conditions, the density of the beam is approximately $8\text{e}16 \text{ m}^{-3}$. The target is 12 mm x 12 mm x 2 mm in size with an initial density of $2\text{E}19 \text{ m}^{-3}$ represented by 576,000 macroparticles of weight $1\text{E}7$ neutrals per macroparticle. Based on these conditions, the

collisional mean free path is 93.45 mm for singly charged ions and 212 mm for doubly charged ions. Since the dimension of the target box parallel to the beam direction is 2 mm, it is highly unlikely that a source particle would undergo more than one collision.

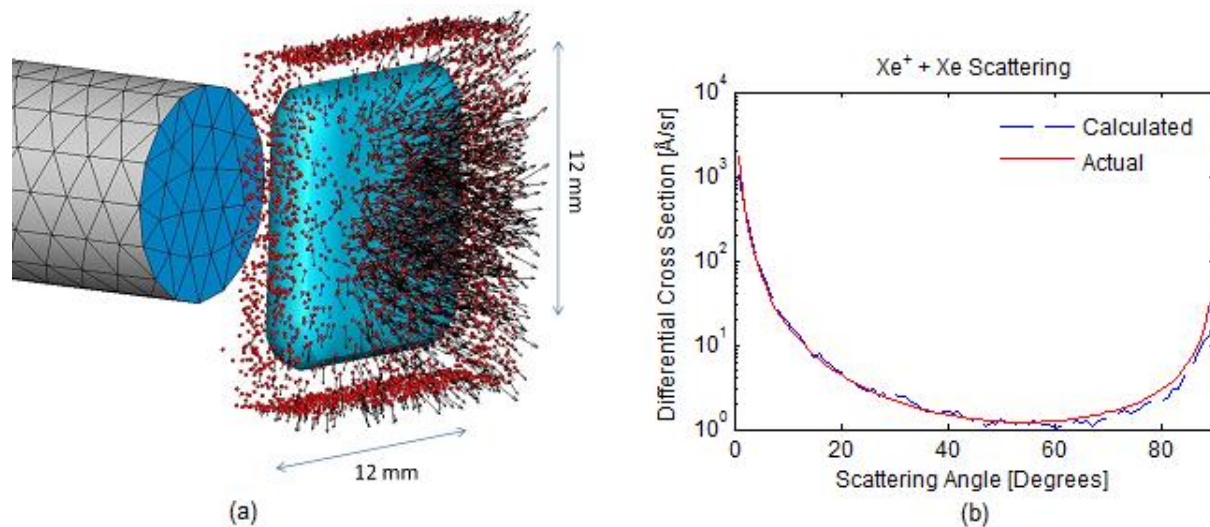


FIGURE 3. Coliseum test case (a) geometry and (b) comparison of calculated and imposed differential cross section.

The position and velocity information of all particles crossing a sample box of size 16 mm x 16 mm x 6 mm around the target is stored for post-processing. The velocity information of the sampled ions is used to calculate a scattering angle for each particle which is binned to generate the calculated differential cross section. This profile is normalized to the published differential cross section at 45 degrees. As shown in Fig. 3(b), the generated differential behavior is consistent with the imposed differential cross section.

SUMMARY

Using published differential cross section data for xenon ions colliding with neutral xenon, a technique has been developed to utilize this data in an existing electric propulsion code, COLISEUM. The data has been pre-processed to be consistent with published total cross section values and to isolate the contributions due to elastic and charge exchange collisions, as well as for computational speed.

ACKNOWLEDGMENTS

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11-15 July 10

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Overview



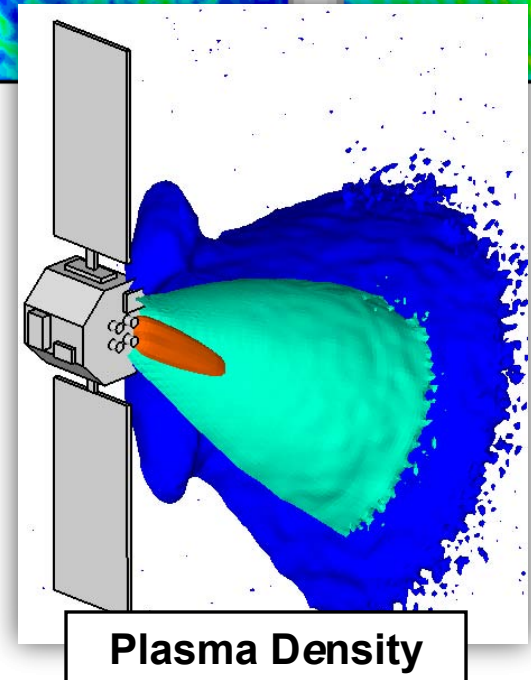
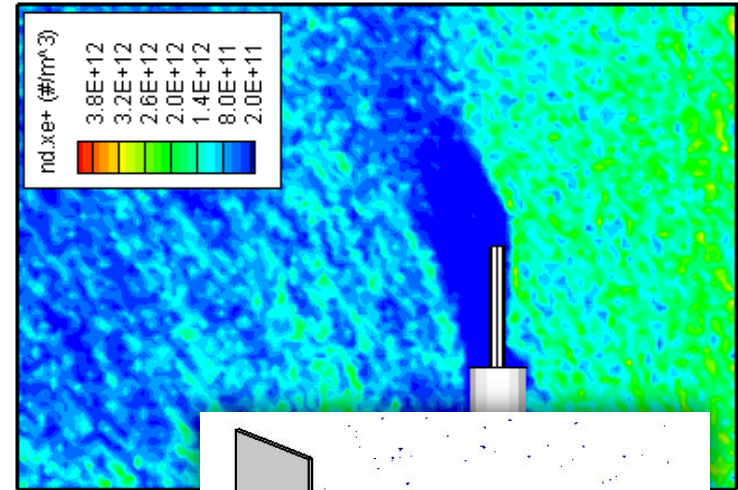
- **Introduction**
- **Differential Cross Section**
- **Monte Carlo Methods**
- **Testing Collision Routines**
- **Summary**



Introduction

- **Motivation for Electric Propulsion Modeling**
 - Understand device physics
 - Thruster optimization
 - Spacecraft integration
- **Collision Models**
 - Collisions important for understanding sputtering and deposition
 - Before: Isotropic scattering and simple charge transfer
 - Now: Based on published differential cross sections [1]

[1] Chiu, Dressler, et al. "Large-angle xenon ion scattering in Xe-propelled electrostatic thrusters: differential cross sections," JOP D, 41, 165503, 2008.



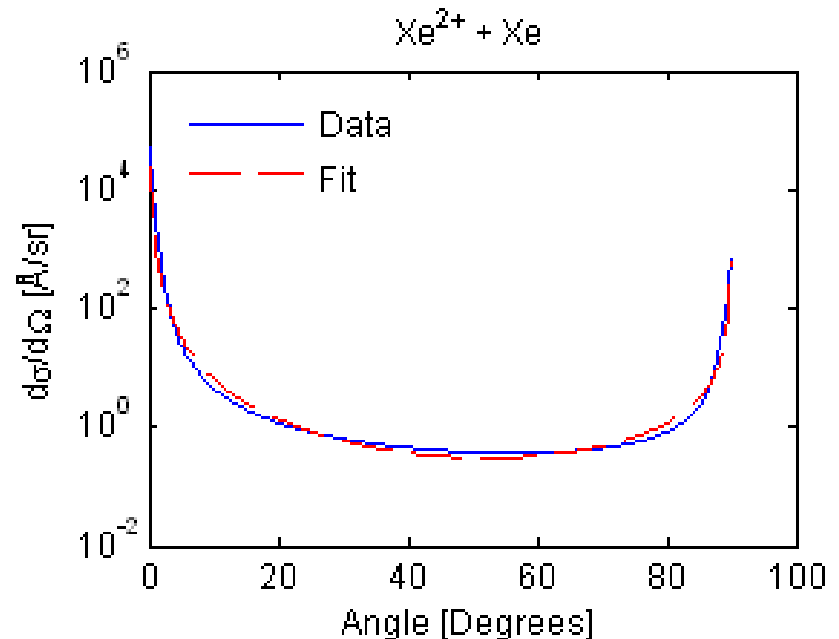
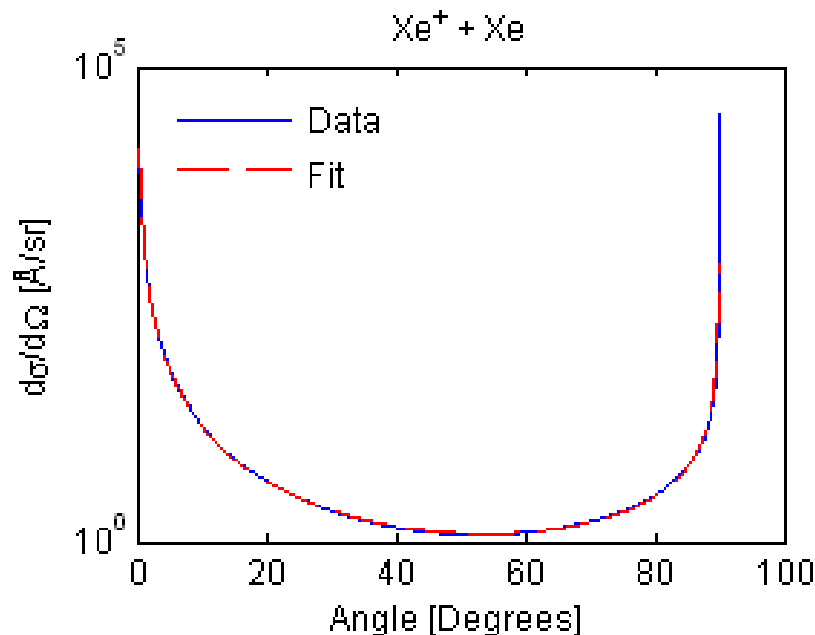
Plasma Density



Differential Cross Section: Fitting a Curve to Published Data

- Xe ion/neutral differential cross section published by Chiu, et al.
- First step: Fit a curve to published data (300 eV)
 - Increased computational speed
 - Allows separation of elastic and charge transfer contributions

$$\left. \frac{d\sigma}{d\Omega} \right|_{LAB} = \theta^{A-el} 10^{B-el} + (90 - \theta)^{A-ct} 10^{B-ct}$$

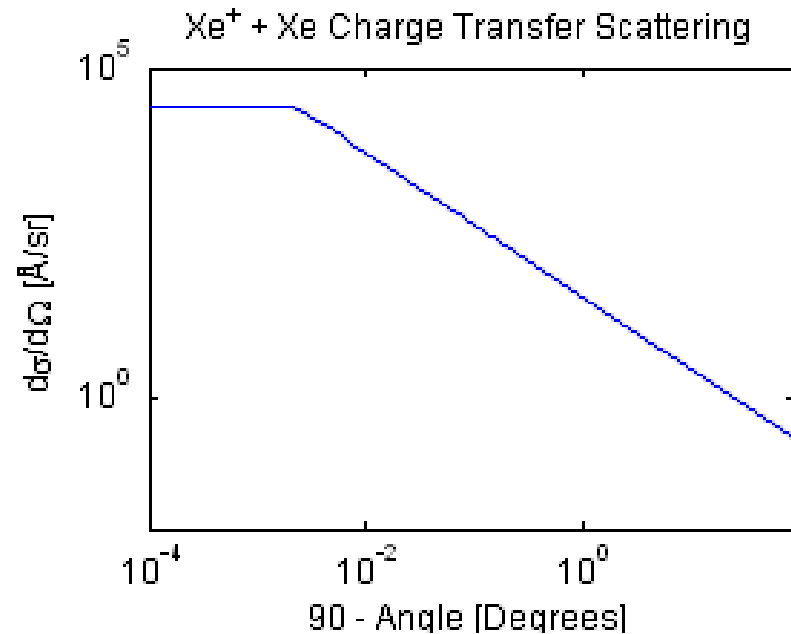
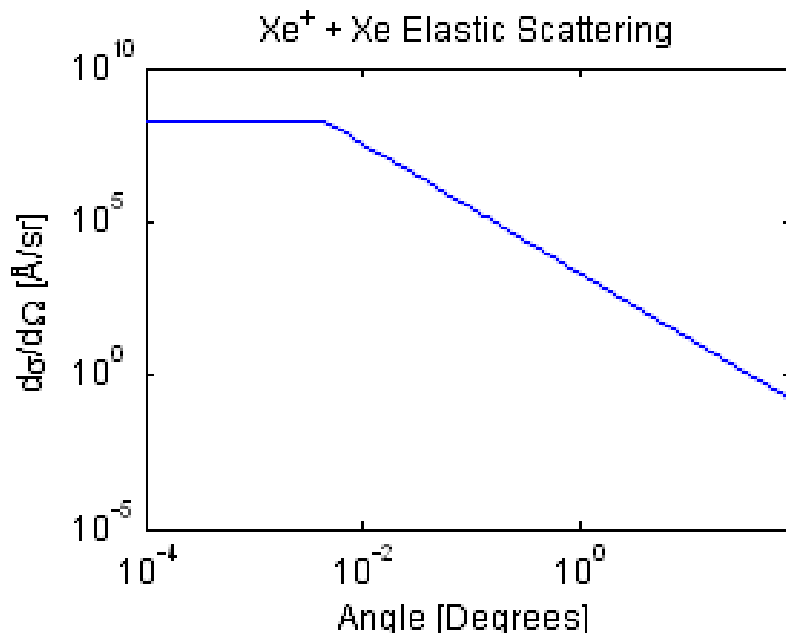




Differential Cross Section: Determining Cutoff Angle

- Published data does not contain information below 0.3 degrees or above 89.95 degrees.
- Second step: Use published total cross section values to determine cutoff angle[2]:

$$\sigma_{tot} = \int_0^\pi \frac{d\sigma}{d\Omega} \bigg|_{LAB} 2\pi \sin(\theta_{rad}) d\theta_{rad}$$



[2] Miller, Pullins, et al., "Xenon charge exchange cross sections for electrostatic thruster models," Journal of Applied Physics, **91**, 3, 2002.



Differential Cross Section: Converting to Center of Mass Frame



- Easier to perform rotations in center of mass frame
- Also, makes differential cross section more meaningful when applied to dissimilar collision partners
- Third step: Convert differential cross section to center of mass coordinates

$$\left. \frac{d\sigma}{d\Omega} \right|_{CM} = \left. \frac{d\sigma}{d\Omega} \right|_{LAB} \frac{1}{4 \cos \theta}$$

$$\chi = 2\theta$$

where θ is the lab frame scattering angle and χ is the center of mass frame scattering angle.



Differential Cross Section: Final Form



- In order to use differential cross section to choose scattering angle, convert solid angle to center of mass scattering angle.

$$\frac{d\sigma}{d\chi} = \frac{d\sigma}{d\Omega}\bigg|_{CM} 2\pi \sin \chi$$

- Final form of differential cross section:

$$\frac{d\sigma}{d\chi} = \begin{cases} \left(\frac{\chi}{2}\right)^{A_{-el}} 10^{B_{-el}} \pi \sin\left(\frac{\chi}{2}\right) & \text{for } \chi \geq 2\theta_{-el} \\ (\theta_{-el})^{A_{-el}} 10^{B_{-el}} \pi \sin(\theta_{-el}) & \text{for } \chi < 2\theta_{-el} \end{cases}$$

$$\frac{d\sigma}{d\chi} = \begin{cases} \left(\frac{\chi}{2}\right)^{A_{-ct}} 10^{B_{-ct}} \pi \cos\left(\frac{\chi}{2}\right) & \text{for } \chi \geq 2\theta_{-ct} \\ (\theta_{-ct})^{A_{-ct}} 10^{B_{-ct}} \pi \cos(\theta_{-ct}) & \text{for } \chi < 2\theta_{-ct} \end{cases}$$



Monte Carlo Methods: Choosing Collision Partners



- **Several mechanisms for choosing collision partners**
 - Calculate the probability of each source particle colliding based on target density (COLISEUM):
$$P = 1 - \exp(-n\sigma|\vec{c}_r|\Delta t)$$
 - Use a no-time-counter method to randomly pick appropriate number of pairs (HPHall).
- **Once collision partners have been chosen:**
 - Azimuthal scattering angle is chosen uniformly: $0 < \phi < 2\pi$
 - Use differential cross section equations to choose polar scattering angle.
 - Apply scattering angles to initial velocity vectors to determine post-collision velocities.



Monte Carlo Methods: Choosing Scattering Angles



- To apply statistical sampling from differential cross section, first choose a comparison function:

$$f_t(\chi) = \begin{cases} \theta^A & \text{for } \chi \leq \theta \\ \chi^A & \text{for } \chi > \theta \end{cases}$$

- Then randomly pick an angle, χ , from comparison function using cumulative distribution function method.

$$\frac{\int_0^\chi f_t(\alpha) d\alpha}{\int_0^\pi f_t(\alpha) d\alpha} = \xi$$

Where ξ is a random number: $0 < \xi < 1$

- Use an acceptance-rejection technique to decide whether or not to retain the selected angle or choose again.



Monte Carlo Methods: Calculating Post-Collision Relative Velocity

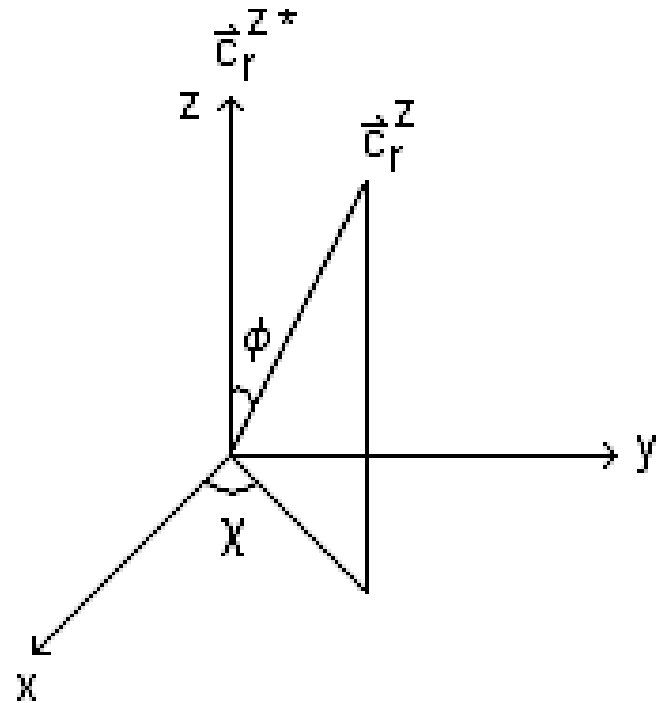


- For simplicity, assume that the pre-collision relative velocity was aligned with a principal-axis, such as z .
- Calculate the post-collision relative velocity in this rotated reference frame:

$$c_{rx}^{z*} = c_r^z \sin \chi \cos \phi$$

$$c_{ry}^{z*} = c_r^z \sin \chi \sin \phi$$

$$c_{rz}^{z*} = c_r^z \cos \chi$$





Monte Carlo Methods: Rotating Coordinate Frame



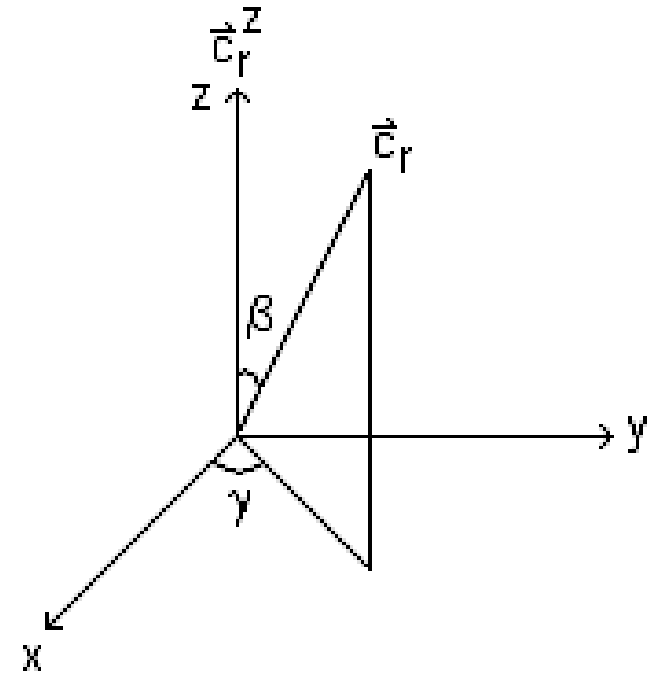
- To account for altered reference frame, first calculate rotation angles to align pre-collision relative velocity vector with principle direction:

$$\beta = \tan^{-1}\left(\sqrt{c_x^2 + c_y^2}\right)$$

$$\gamma = \tan^{-1}\left(\frac{c_y}{c_x}\right)$$

- Rotate post-collision relative velocity vector according to rotation angles:

$$\vec{c}_r^* = \begin{bmatrix} \cos \gamma & -\sin \gamma & 0 \\ \sin \gamma & \cos \gamma & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} \cos \beta & 0 & \sin \beta \\ 0 & 1 & 0 \\ -\sin \beta & 0 & \cos \beta \end{bmatrix} \vec{c}_r^{z*}$$





Monte Carlo Methods: Converting to Laboratory Frame



- Lastly, convert back to laboratory reference frame from center of mass reference frame:

$$\vec{c}_{source}^* = \vec{c}_m + \frac{m_{target}}{m_{source} + m_{target}} \vec{c}_r^*$$

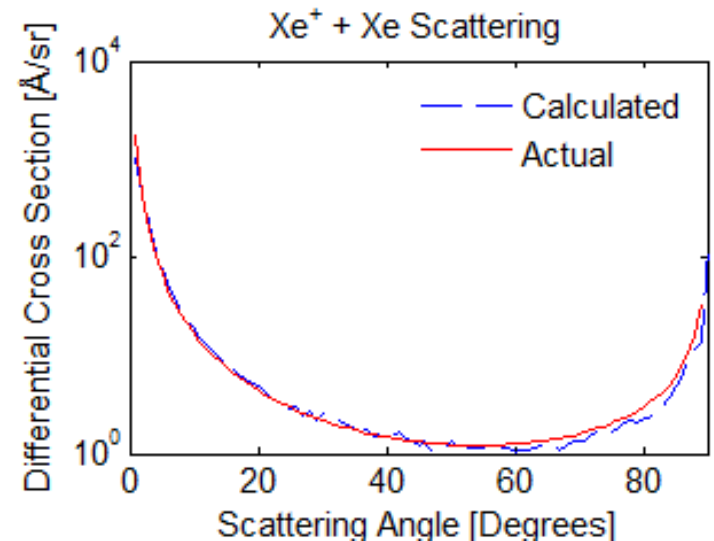
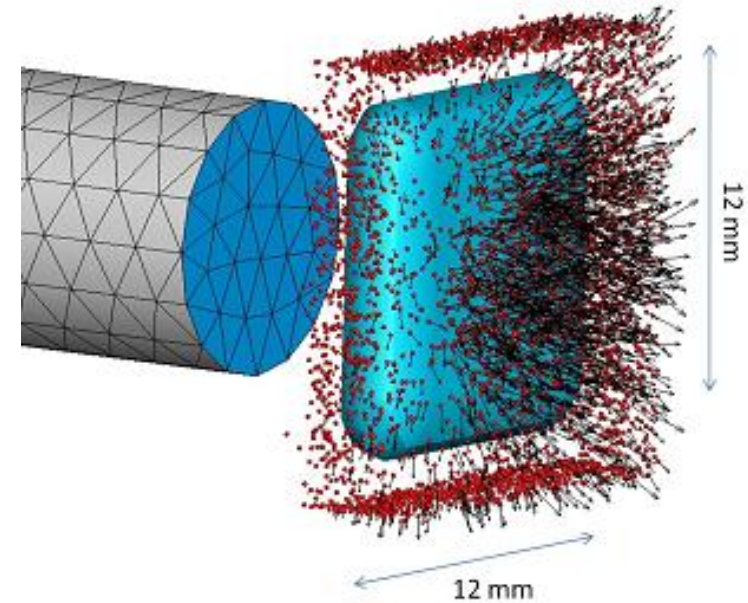
$$\vec{c}_{target}^* = \vec{c}_m - \frac{m_{source}}{m_{source} + m_{target}} \vec{c}_r^*$$

- In the case of charge transfer collisions, the source and target particle identities are exchanged after the new velocities have been calculated.



COLISEUM Test Case

- **COLISEUM is an electric propulsion plume model using hybrid techniques with PIC heavy particles**
- **Generate simple case in COLISEUM to test collision routines**
 - Injector: Xe^+ , 10 mm diameter, 300 eV, 100 K, $2.78\text{e-}8$ kg/s, $8\text{E}16$ m⁻³
 - Target cell: 12 mm x 12 mm x 2 mm, 576,000 macroparticles, $2\text{E}19$ m⁻³
 - Mean Free Path: 93.45 mm
- **Sample ions crossing a box (16 mm x 16 mm x 6 mm) around target cell**
- **Angular distribution of sampled ions is consistent with imposed differential cross section**





Summary



- **Differential cross section data for collisions between xenon ions and neutral xenon has recently been published.**
- **This new data allows for more accurate predictions of post-collision products.**
- **The published differential cross section has been simplified and pre-processed for use in existing electric propulsion models.**
- **Simple test case in electric propulsion plume code, COLISEUM, verifies proper implementation.**
- **Using the new collision data allows for more accurate predictions of the interactions between the high velocity ions leaving the device and the slow-moving neutral plume of exhaust.**
 - Provides more accurate calculation of high angle fluxes
 - Improves spacecraft integration modeling